Group of Carbon Nanostructures and Nanotechnology

INSTITUTO DE CARBOQUÍMICA

Formation of P3HT aggregates enhanced by type-II cellulose nanocrystals

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Introduction

Poly-3-hexylthiophene (P3HT) is one of the most studied structures for optoelectronic devices because of its charge transport ability and photocurrent generation in solar cells. Previous studies have noticed the increasing formation of J-aggregates in some hybrid materials when P3HT nanoparticles are synthetized in presence of other nanostructures like graphene oxide[1].

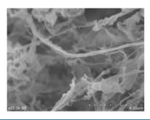
Nanocrystalline cellulose (NCC) is a very promising new material because it comes from one of the most abundant source in nature. Moreover, NCC can be synthetized in different crystalline forms. While type I has been widely studied, works with type II NCC are scarcely reported.

In this work, we have synthetized a new hybrid material, consisting on P3HT-NCC(II) nanoparticles where J-aggregates formation in polythiophene species is greatly improved.

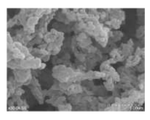
[1] Istif, E.; Hernández-Ferrer, J.; Urriolabeitia, E. P.; Stergiou, A.; Tagmatarchis, N.; Fratta, G.; Large, M. J.; Dalton, A. B.; Benito, A. M.; Maser, W. K. *Adv. Func. Mat.* **2018**, 28 (23), 1707548.

NCC comparative

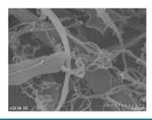
NCC I



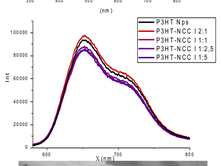
P3HT



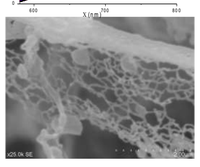
NCC II



Almost no effect observed, **even with concentrations 10 times higher**



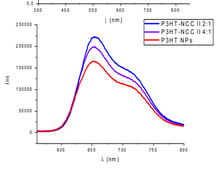
Fluorescence spectra remain roughly unalterable with the addition of NCC I



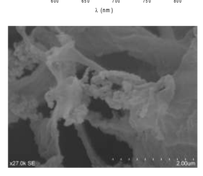
In SEM microscopy, polymer nanoparticles seem to be trapped on a NCC I wire

P3HT and NCC I barely interact

Important changes in spectra, resulting in a sample **color change**



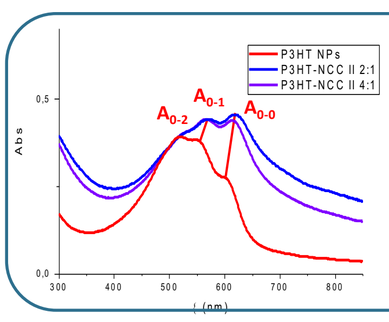
Fluorescence is enhanced by the NCC II presence



In SEM microscopy, polymer nanoparticles apparently grow along NCC II crystals

Strong interaction between P3HT and NCC II

J-Aggregates enhancement with NCC II

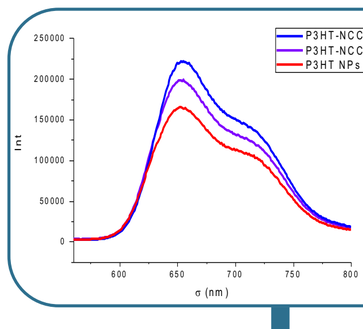


Remarkable change in the absorbance ratio between transitions $A_{0\text{-}0}$ and $A_{0\text{-}1}$

Absorption peaks are redshifted

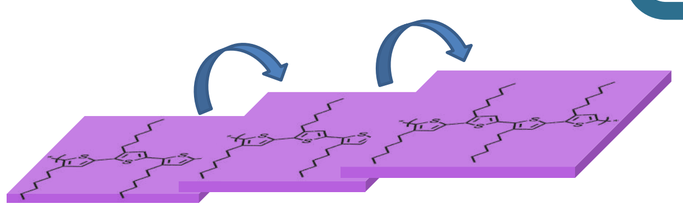
$$\frac{A_{0-0}}{A_{0-1}} = \frac{\left(1 - 0.96J_0/E_p\right)^2}{\left(1 + 0.292J_0/E_p\right)^2}$$

J_o is null or even negative



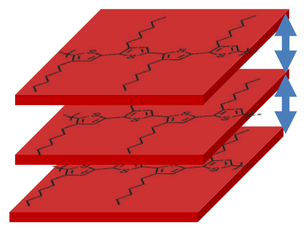
Increasing fluorescence with larger amount of NCC II

J-Aggregates



J- Aggregates dominate over H-Aggregates

H-Aggregates



Conclusions

We have synthetized for the first time a new hybrid P3HT nanoparticles in presence of two crystalline types of NCC and demonstrated a highly promoted interaction with NCC(II) while NCC(I) seem to be barely inactive when P3HT nanoparticles formation takes place.

This nanomaterial has increased J-aggregates in its structure with a rising fluorescence correlated to the amount of NCC (II) in the sample and could offer a promising new applications in optoelectronic devices.

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